CATEGORIZATION OF UCVBS USING CHEMICAL-BIOLOGICAL READ ACROSS

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RATIONALE

Aims to provide a method for predicting the biological activity of substances not yet tested, based on the analysis of existing data from existing data collection. The process involves the integration of a large body of existing data from various sources, including experimental and computational methods, to develop a comprehensive understanding of the biological effects of a wide range of substances. The method is based on the principle that substances with similar chemical structures are likely to have similar biological effects. The method involves the use of a combination of computational and experimental approaches to predict the biological activity of substances not yet tested.

WORKFLOW

1. Identification of relevant data sources
2. Data preprocessing
3. Data analysis
4. Model development
5. Model validation
6. Model application

RESULTS

ION MOBILITY-MASS SPECTROMETRY

Chemical Composition-Based Grouping of Petroleum Substances

PHENOTYPIC IN VITRO SCREENING

Biological Data- Integrative Compendium of Petroleum Substances

DIFFERENTIAL GENE EXPRESSION IN PETROLEUM-SUBSTANCE-TREATED ISPC HEPATOMA CELLS

CONCLUSIONS

- The method can be used to predict the biological activity of substances not yet tested, based on the analysis of existing data from existing data collection. The process involves the integration of a large body of existing data from various sources, including experimental and computational methods, to develop a comprehensive understanding of the biological effects of a wide range of substances. The method is based on the principle that substances with similar chemical structures are likely to have similar biological effects. The method involves the use of a combination of computational and experimental approaches to predict the biological activity of substances not yet tested.

- The results of the method can be used to identify substances with similar biological effects, which can be useful for risk assessment and regulatory purposes. The method can also be used to identify substances with attractive or adverse biological effects, which can be useful for the development of new substances or the modification of existing substances.

- The method can be used to identify substances with potential therapeutic applications, which can be useful for the development of new drugs or the modification of existing drugs.

FUTURE WORK

- The method can be further developed to include additional data sources and to improve the accuracy of the predictions.

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REFERENCES

QR-CODE

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